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TWELFTH REPORT ON  
A SURVEY OF THERMODYNAMIC PROPERTIES OF THE  
COMPOUNDS OF THE ELEMENTS CHNOPS

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and Martin L. Reilly

Progress Report for the Period 1 April to 30 June 1967

to

National Aeronautics and Space Administration

Contract No. R-138, Amendment 2.

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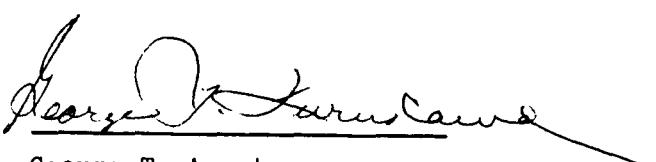
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## FOREWORD

A study at the National Bureau of Standards (NBS), of which this is the twelfth progress report, has been undertaken to meet the need of the National Aeronautics and Space Administration (NASA) for thermodynamic information on biologically related materials important to the space program for several reasons. Among these reasons are the necessity of inferring the maximum account of useful chemistry of incompletely accessible environments, for which only limited information is available, the possibility of the occurrence of organic compounds naturally synthesized under primitive conditions, and the possibility of theoretically recovering part of the prebiological history of the earth.

This program is being carried out under the technical supervision of Dr. George Jacobs of NASA, and with the consultation of Dr. Harold Morowitz of the Yale University, Department of Molecular Biology and Biophysics, and Dr. C. W. Beckett of the Heat Division, Institute for Basic Standards (NBS). The contract (Contract No. R-138) was initiated 1 May 1964 and extended by Amendments 1 and 2. This report covers the third quarter of the work being carried out under Amendment 2.

for

  
George T. Armstrong  
Supervisory Chemist  
Project Leader

## Section I.

### Analysis of Heat-Capacity Data

Martin L. Reilly and George T. Furukawa

This report gives the details of the results obtained in the analysis of heat-capacity data on normal aliphatic hydrocarbons containing from 8 to 16 carbons and on tetraphosphorus decasulfide ( $P_4S_{10}$ ). A preliminary brief summary of the results was reported earlier (see Eleventh Report on a Survey of Thermodynamic Properties of the Compounds of the Elements CHNOPS, National Bureau of Standards Report No. 9553, June 15, 1967).

In the following sections the sources of heat-capacity data for each of the substances are discussed and the interpretations of the experimental data are compared. The values of mean heat capacity for the temperature interval 0° to 50°C on the  $C_8$  to  $C_{16}$  hydrocarbons, reported in 1902 by Mabery and Goldstein [4]<sup>1</sup>, were considered to be only of historical interest and were not given any weight in the analysis.

The tables of thermodynamic properties obtained for the n-aliphatic hydrocarbons from  $C_8$  to  $C_{16}$  and for  $P_4S_{10}$  are given at the end of this section.

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<sup>1</sup> The numbers in brackets represent the literature references given at the end of this section.

n-Octane, C<sub>8</sub>H<sub>18</sub>

The analysis was based largely on the experimental heat-capacity data reported by Finke, et al. [2], from 13° to 298°K. Premelting corrections were applied to the data above 230°K by using the impurity content (0.06 mole percent) estimated by Finke, et al. [2]. The solid-phase heat-capacity data were extrapolated to 0°K using the equation  $C_s = 7R \times D(134/T)^a$  given by Finke, et al. No transition or anomaly has been observed in the solid phase. The triple-point temperature was taken to be 216.38°K and the heat of fusion to be 4957 cal/mole [2].

The liquid-phase data were found to be represented best by a cubic equation. The estimated standard deviation of the observed data from the cubic equation is ±0.018 cal/deg-mole (±0.03 percent of the average liquid-phase heat capacity for the temperature interval of the measurements).

The data on n-octane published by Parks, et al. [6] and Huffman, et al. [3] are based upon samples of lower estimated purity. Their data, therefore, were given less weight. The observations (283 to 308°K) of Osborne and Ginnings [5] in the liquid phase are in good agreement with those of Finke, et al. [2].

The entropy at 298.15°K ( $S_{298}^0$ ) that has been obtained from the data analysis for liquid n-octane at the saturation pressure compares with other published values as follows:

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<sup>a</sup>  $D(134/T)$  represents the Debye heat-capacity function with the characteristic temperature 134°K.

<u>Year</u>	<u>S<sub>298</sub><sup>o</sup></u>	
	<u>cal/deg-mole</u>	
1930	86.0	Parks, <u>et al.</u> [6]
1931	86.0	Huffman, <u>et al.</u> [3]
1953	86.326 ±0.17	Finke, <u>et al.</u> [2]
1967	86.30 ±0.20	[This work]

n-Nonane, C<sub>9</sub>H<sub>20</sub>

The experimental measurements (12 to 314°K) reported by Finke, et al. [2] were used as the main basis of this analysis. Premelting corrections were applied to the solid-phase data above 140°K using the estimated impurity content (0.12 mole percent) given by Finke, et al. [2]. The solid-phase data were extrapolated to 0°K using the equation  $C_s = 7R \times D(129.5/T)$  given by Finke, et al. [2]. In the range 20° to 60°K and just below the transition point, a slightly different interpretation was placed upon the solid-phase heat capacity, resulting in somewhat lower smoothed values in each case. The solid-phase transition temperature was taken to be 217.19°K and the heat of transition to be 1510 cal/mole. (This is the sum of 1501 cal/mole reported by the above authors plus 9 cal/mole arising from the difference in the smoothed heat capacities above 160°K mentioned earlier.)

The heat of fusion was taken to be 3697 cal/mole and the triple-point temperature to be 219.66°K. The liquid-phase heat capacity can be represented best by a cubic equation. The estimated standard deviation of the observed values from the equation is ±0.022 cal/deg-mole (approximately ±0.03 percent of the mean liquid heat capacity of the interval of

observations). The data of Osborne and Ginnings (278 to 318°K) [5] are in excellent agreement with the final selected values.

The heat-capacity data reported by Parks, et al. [6] and by Huffman, et al. [3] were obtained with far less pure samples and were found to be significantly lower than those reported by Finke, et al. [2] and Osborne and Ginnings [5] (approximately 0.2 to 0.4 percent).

The entropy at 298.15°K that has been obtained from the analysis for liquid n-nonane at the saturation pressure compares with other published values as follows:

<u>Year</u>	$S_{298}^0$ <u>cal/deg-mole</u>	
1930	93.9	Huffman, <u>et al.</u> [3]
1953	94.091 ±0.19	Finke, <u>et al.</u> [2]
1967	94.06 ±0.30	[This work]

#### n-Decane, C<sub>10</sub>H<sub>22</sub>

The heat-capacity measurements between 12° and 319°K reported by Finke, et al. [2] on a sample of 99.91 mole-percent purity have been used as the main basis for this analysis. In the range 160° to 210°K, the heat-capacity data exhibit an anomalous behavior. The data published earlier by Huffman, et al. [3] for a sample of lower purity (judged on the basis of a larger "premelting effect" indicated by the data) do not show such a behavior. Finke, et al. [2] attributed the anomaly to impurity and excluded the contribution of the anomaly from the heat capacity. The same procedure was followed in the present analysis. Premelting corrections were applied to the observed data in the region below the triple-point

temperature. A cubic equation was fitted to 10 data points between 150° and 230°K after eliminating those data points that were obviously part of the anomaly. The heat capacities thus obtained are somewhat lower; therefore, the entropy increment over the temperature interval is slightly lower (0.020 cal/deg-mole) than that estimated from the smoothed values of heat capacity given by Finke, et al. [2].

The solid-phase heat capacity was extrapolated to 0°K using the equation  $C_s = 8R \times D(137.1/T)$ . The heat of fusion was taken to be 6863 cal/mole and the triple-point temperature to be 243.51°K.

The liquid-phase heat capacity reported by Finke, et al. [2] was found to be represented best by a cubic equation. The estimated standard deviation of the data from the equation is  $\pm 0.016$  cal/deg-mole ( $\pm 0.02$  percent of the mean liquid-phase heat capacity for the interval of measurements). The data reported by Osborne and Ginnings [5] between 278° and 318°K are in good agreement with the final selected values of heat capacity. The values reported by Parks, et al. [6] and Huffman, et al. [3] deviate considerably.

The entropy at 298.15°K that has been obtained from the analysis for liquid n-decane at the saturation pressure compares with other published values as follows:

<u>Year</u>	$S_{298}^{\circ}$ <u>cal/deg-mole</u>	
1931	102.5	Huffman, <u>et al.</u> [3]
1953	101.793 $\pm 0.20$	Finke, <u>et al.</u> [2]
1967	101.77 $\pm 0.25$	[This work]

n-Undecane, C<sub>11</sub>H<sub>24</sub>

The experimental data (12 to 299°K) of Finke, et al. [2] were used for the analysis. Premelting corrections were applied to the observed data using the estimated impurity content (0.02 mole percent) reported by Finke, et al. [2]. The data were extrapolated to 0°K using the equation  $C_s = 7R \times D(124.9/T)$  given by Finke, et al. [2]. A few data points in the region 110° to 130°K indicate a lack of thermal equilibrium in the solid phase; otherwise, the data are well behaved. The analysis of the data from 12° to 220°K produced, in general, slightly higher smoothed heat capacities than those obtained by Finke, et al. [2]; therefore, the entropy at 220°K is approximately 0.020 cal/deg-mole higher.

The heat of transition was taken to be 1639 cal/mole and the transition temperature to be 236.6°K.

The observed heat capacities between 236.6° and 247.59°K were fitted by a straight line and then adjusted slightly to conform with the entropy increment obtained by Finke, et al. [2] for the temperature interval.

The heat of fusion was taken to be 5301 cal/mole and the triple-point temperature to be 247.59°K.

The observed liquid-phase data were fitted by a cubic equation. The estimated standard deviation of the observed values from the equation is ±0.034 cal/deg-mole (equivalent to ±0.02 percent of the average liquid-phase heat capacity for the interval of observations).

The entropy at 298.15°K that has been obtained from the analysis for liquid n-undecane at the saturation pressure compares with other published values as follows:

<u>Year</u>	$S_{298}^{\circ}$	
	<u>cal/deg-mole</u>	
1931	110.9	Huffman, <u>et al.</u> [3]
1953	109.495 ±0.22	Finke, <u>et al.</u> [2]
1967	109.53 ±0.25	[This work]

n-Dodecane, C<sub>12</sub>H<sub>26</sub>

The experimental heat-capacity measurement (12 to 317°K) reported by Finke, et al. [2] are the basis for this analysis. The data published by Huffman, et al. [3] were obtained for a sample of significantly lower purity; they, therefore, were not given any weight. The observed heat capacity dat were corrected wherever significant for premelting using the impurity content (0.07 mole percent) given by Finke, et al. [2]. The solid-phase heat capacity was extrapolated to 0°K using the equation  $C_s = 8R \times D(132.3/T)$  reported by Finke, et al. [2]. The smoothed heat capacities obtained for the interval 20 to 110°K are generally higher than those published by Finke, et al. [2] and the entropy at 110°K is correspondingly higher by about 0.020 cal/deg-mole. In addition, the smoothed heat capacities in the region below the triple-point temperature given by Finke, et al. [2] closely follow the observed data that have not been corrected for premelting effects. The entropy obtained for the solid at the triple-point temperature is 0.031 cal/deg-mole lower than the value reported by Finke, et al. [2].

The heat of fusion and the triple-point temperature were taken to be those given by Finke, et al. [2], 8804 cal/mole and 263.59°K, respectively.

The liquid-phase observed heat capacities were fitted to a cubic equation. The estimated standard deviation of the observed data from the equation is  $\pm 0.030$  cal/deg-mole (corresponding to  $\pm 0.03$  percent of the average observed liquid-phase heat capacity).

The entropy at 298.15°K that has been obtained from the analysis for liquid n-dodecane at the saturation pressure compares with other published values as follows:

<u>Year</u>	$S_{298}^{\circ}$	
	<u>cal/deg-mole</u>	
1931	118.1	Huffman, <u>et al.</u> [3]
1953	117.267 $\pm 0.23$	Finke, <u>et al.</u> [2]
1967	117.25 $\pm 0.30$	[This work]

#### n-Tridecane, C<sub>13</sub>H<sub>28</sub>

The experimental measurements (12 to 306°K) reported by Finke, et al. [2] are the basis of this analysis. The estimated impurity content of the sample was 0.05 mole percent. Premelting corrections were applied to the solid-phase data below the triple-point temperature. The data were extrapolated to 0°K using the equation  $C_s = 8R \times D$  ( $126.5/T$ ) given by Finke, et al. [2]. In the region just below the solid-phase transition, an adjustment was made to the distribution of energy between the heat capacity and the transition, resulting in

slightly lower smoothed heat capacities than those reported by Finke, et al. [2]. The heat of transition was correspondingly increased by 12 cal/mole to a new value of 1843 cal/mole. The transition temperature was taken to be 255.05°K.

The observed data between the transition and triple-point temperatures were fitted by a straight line with an estimated standard deviation corresponding to about 0.3 percent of the average value of heat capacity for the phase. The heat of fusion was taken to be 6812 cal/mole and the triple-point temperature to be 267.79°K. The liquid-phase heat-capacity data are represented by a quadratic equation with an estimated standard deviation of the observed data from the equation of 0.048 cal/deg-mole ( $\pm 0.05$  percent of the average liquid-phase heat capacity between 268 and 310°K).

The entropy at 298.15°K that has been obtained from the data analysis for liquid n-tridecane at the saturation pressure compares with the value reported by Finke, et al. [2] as follows:

<u>Year</u>	$S_{298}^{\circ}$	
	<u>cal/deg-mole</u>	
1953	124.966 $\pm 0.25$	Finke, <u>et al.</u> [2]
1967	124.96 $\pm 0.30$	[This work]

#### n-Tetradecane, C<sub>14</sub>H<sub>30</sub>

Experimental heat-capacity measurements (12 to 303°K) reported by Finke, et al. [2] are the basis of this analysis. The measurements (93 to 291°K) reported by Parks and Light [7] on a sample of considerably lower purity were not given any weight. Premelting corrections were applied

to the solid-phase data using the impurity content (0.07 mole percent) reported for the sample by Finke, et al. [2]. The data were extrapolated to 0°K using the equation  $C_s = 8.5 R \times D(131.1/T)$  given by Finke, et al. [2]. The solid-phase heat capacity was found to be well behaved, free of any anomalies.

The smoothed values of heat capacity published by Finke, et al. [2] generally tend to be higher than their experimental values below 100°K. The entropy at 100°K that has been obtained is, therefore, 0.015 cal/deg-mole lower than that of Finke, et al. [2].

The heat of fusion was taken to be 10772 cal/mole and the triple-point temperature to be 279.03°K.

The liquid-phase heat-capacity data were fitted to a straight line with an estimated standard deviation of the observed values from the equation of  $\pm 0.037$  cal/deg-mole ( $\pm 0.04$  percent of the average liquid-phase heat capacity in the interval).

The entropy at 298.15°K that has been obtained from the data analysis for liquid n-tetradecane at the saturation pressure compares with other published values as follows:

<u>Year</u>	$S_{298}^o$ <u>cal/deg-mole</u>	
1934	134.4	Parks and Light [7]
1953	132.746 $\pm 0.26$	Finke, <u>et al.</u> [2]
1967	132.73 $\pm 0.30$	[This work]

n-Pentadecane, C<sub>15</sub>H<sub>32</sub>

The experimental heat-capacity measurements (12 to 313°K) reported by Finke, et al. [2] are the basis of this analysis. Premelting corrections were applied to the solid-phase data based on the impurity content (0.05 mole percent). The data were extrapolated to 0°K using the equation  $C_s = 9R \times D(130.2/T)$  given by Finke, et al. [2]. As with n-tetradecane, the smoothed values obtained by Finke, et al. [2] are generally higher than their observed values for temperatures below 150°K. The entropy obtained at 150°K is, therefore, about 0.023 cal/deg-mole lower than that of Finke, et al. [2].

In the interval 230 to 270°K, the distribution of energy between heat capacity and heat of transition has been slightly adjusted, resulting in lower values for heat capacity and a higher heat of transition. The heat of transition was taken to be 2214 cal/mole which is 23 cal/mole higher than the value reported by Finke, et al. [2]. The transition temperature was taken to be 270.90°K.

The solid-phase heat capacities between the transition and triple-point temperatures were fitted with a straight line with an estimated standard deviation of ±0.188 cal/deg-mole (±0.15 percent of the average heat capacity of the phase).

The heat of fusion was taken to be 8268 cal/mole and the triple-point temperature to be 283.11°K.

The liquid-phase heat capacities were fitted with a quadratic equation with an estimated standard deviation of ±0.023 cal/deg-mole (±0.02 percent of the average liquid-phase values for the temperature interval of the measurements reported).

The entropy at 298.15°K that has been obtained from the data analysis for liquid n-pentadecane at the saturation pressure compares with the value reported by Finke, et al. [2] as follows:

<u>Year</u>	$S_{298}^o$ <u>cal/deg-mole</u>	
1953	140.416 ±0.28	Finke, <u>et al.</u> [2]
1967	140.38 ±0.30	[This work]

n-Hexadecane, C<sub>16</sub>H<sub>34</sub>

The experimental heat-capacity measurements (12 to 320°K) reported by Finke, et al. [2] are the basis of this analysis. The data (80 to 300°K) reported by Parks, et al. [8] on a sample estimated to be 95 mole-percent pure were not given any weight. Premelting corrections were applied to the solid-phase data based on the impurity content (0.12 mole percent) found by Finke, et al. [2]. The solid-phase data were extrapolated to 0°K using the equation  $C_s = 9R \times D(129.6/T)$ . No transitions or anomalies were observed in the solid phase. An inconsistency was found in the treatment of the data by Finke, et al. [2] in the premelting region. Their smoothed values are significantly higher than the observed data corrected for premelting. The smoothed values of heat capacity obtained in the present analysis are consistent with the observed values corrected for premelting. The entropy of the solid phase at the triple-point temperature, 291.34°K, is, therefore, lower by 0.027 cal/deg-mole than the value reported by Finke, et al. [2]. The heat of fusion was taken to be 12753 cal/mole.

The liquid-phase heat-capacity data were fitted by a quadratic equation with an estimated standard deviation of  $\pm 0.038$  cal/deg-mole ( $\pm 0.03$  percent of the average liquid phase heat capacity over the temperature interval of the measurements).

The entropy at  $298.15^{\circ}\text{K}$  that has been obtained from the analysis for liquid n-hexadecane at the saturation pressure compares with other published values as follows:

<u>Year</u>	$S_{298}^{\circ}$	
	<u>cal/deg-mole</u>	
1949	149.8	Parks, <u>et al.</u> [8]
1953	$148.09 \pm 0.29$	Finke, <u>et al.</u> [2]
1967	$148.07 \pm 0.40$	[This work]

#### Tetraphosphorus Decasulfide, $\text{P}_4\text{S}_{10}$

The experimental values of heat capacity (6 to  $345^{\circ}\text{K}$ ) reported by Clever, et al. [1] are the basis of this analysis. The sample was prepared by purifying a technical-grade material by repeated extraction with carbon disulfide and finally vacuum removal of the solvent.

The data have been found to be very precise except within the region below approximately  $15^{\circ}\text{K}$ . The interpretation of the data below  $15^{\circ}\text{K}$  is slightly different from that of Clever, et al. [1], with the result that the entropy at  $15^{\circ}\text{K}$  was found to be 0.049 cal/deg-mole higher than that calculated by Clever, et al. Above  $15^{\circ}\text{K}$  the analysis closely followed that made by Clever, et al. [1].

The entropy at 298.15°K obtained from the analysis of the heat-capacity data for tetraphosphorus decasulfide compares with that of Clever, et al. [1] as follows:

<u>Year</u>	$S_{298}^{\circ}$	
	<u>cal/deg-mole</u>	
1965	91.24	Clever, <u>et al.</u> [1]
1967	91.29 ±0.20	[This work]

TABLE 121

## MOLAL THERMODYNAMIC FUNCTIONS FOR OCTANE

NORMAL-C<sub>8</sub>H<sub>18</sub>

SOLID AND LIQUID PHASES

T DEG K=273.15+T DEG C

1 CAL=4.1840 JOULES

GRAM MOLECULAR WT.= 114.23266 GRAMS

T DEG K	C <sub>S</sub> CAL DEG MOL	(H <sub>S</sub> -E <sub>0</sub> <sup>C</sup> ) CAL MOL	(H <sub>S</sub> -E <sub>0</sub> <sup>C</sup> )/T DEG MOL	S <sub>S</sub> <sup>0</sup> CAL DEG MOL	-(G <sub>S</sub> -E <sub>0</sub> <sup>C</sup> ) CAL MOL	-(G <sub>S</sub> -E <sub>0</sub> <sup>C</sup> )/T DEG MOL
SOLID TRICLINIC						
3.00	0.000	0.000	0.000	0.000	0.000	0.000
5.00	0.056	0.070	0.014	0.019	0.023	0.005
10.00	0.450	1.128	0.113	0.150	0.376	0.038
15.00	1.437	5.585	0.372	0.498	1.892	0.126
20.00	2.918	16.337	0.817	1.107	5.800	0.290
25.00	4.603	35.091	1.404	1.937	13.330	0.533
30.00	6.359	62.481	2.083	2.931	25.441	0.848
35.00	8.099	98.665	2.819	4.043	42.835	1.224
40.00	9.761	142.35	3.584	5.234	65.999	1.650
45.00	11.342	196.14	4.359	6.475	95.255	2.117
50.00	12.862	256.67	5.133	7.749	130.81	2.616
55.00	14.323	324.66	5.903	9.044	172.78	3.142
60.00	15.885	399.73	6.662	10.350	221.27	3.688
65.00	16.933	481.32	7.405	11.655	276.26	4.251
70.00	18.103	563.93	8.128	12.953	337.81	4.826
75.00	19.236	662.29	8.831	14.241	405.80	5.411
80.00	20.335	761.24	9.515	15.518	480.20	6.003
85.00	21.378	865.55	10.183	16.782	560.96	6.600
90.00	22.348	974.89	10.832	18.032	648.00	7.200
95.00	23.252	1088.9	11.462	19.265	741.25	7.803
100.00	24.109	1207.3	12.073	20.480	840.62	8.406
105.00	24.937	1330.0	12.666	21.676	946.02	9.010
110.00	25.743	1456.7	13.242	22.855	1057.4	9.612
115.00	26.529	1587.3	13.803	24.016	1174.5	10.213
120.00	27.295	1721.0	14.349	25.162	1297.5	10.812
125.00	28.041	1856.3	14.882	26.291	1426.1	11.409
130.00	28.770	2002.3	15.402	27.405	1560.4	12.003
135.00	29.484	2147.9	15.911	28.504	1700.2	12.594
140.00	30.184	2297.1	16.408	29.539	1845.4	13.181
145.00	30.874	2442.8	16.895	30.601	1996.0	13.766
150.00	31.557	2605.8	17.372	31.710	2152.0	14.347
155.00	32.236	2765.3	17.841	32.765	2313.2	14.924
160.00	32.815	2822.2	18.291	32.799	2479.6	15.498
165.00	33.381	3074.5	18.734	34.822	2651.2	16.068
170.00	34.298	3234.3	19.201	35.936	2827.9	16.634
175.00	35.015	3437.5	19.643	36.840	3009.5	17.197
180.00	35.758	3614.4	20.080	37.827	3196.2	17.757
185.00	36.538	3795.1	20.514	38.827	3387.0	18.313
190.00	37.364	3979.0	20.947	39.812	3584.8	18.866
195.00	38.245	4168.0	21.370	41.794	3785.0	19.415
200.00	39.188	4362.4	21.812	41.774	3997.4	19.962
205.00	40.199	4560.9	22.248	42.754	4209.7	20.506
210.00	41.281	4764.5	22.688	43.736	4419.0	21.047
215.00	42.433	4973.8	23.134	44.720	4641.1	21.586
216.38	42.763	5032.6	23.258	45.923	4703.0	21.735
LIQUID PHASE						
216.38	55.515	9989.6	46.167	67.902	4703.0	21.735
220.00	55.551	10191.	46.321	68.823	4950.5	22.502
225.00	55.644	10469.	46.527	70.072	5297.7	23.545
230.00	55.784	10747.	46.727	71.297	5651.1	24.570
235.00	55.968	11027.	46.921	72.498	6010.6	25.577
240.00	56.194	11307.	47.112	73.679	6376.1	26.567
245.00	56.457	11589.	47.300	74.840	6747.4	27.540
250.00	56.755	11872.	47.486	75.984	7124.5	28.498
255.00	57.084	12156.	47.671	77.111	7507.2	29.440
260.00	57.441	12442.	47.855	78.223	7895.6	30.368
265.00	57.823	12731.	48.040	79.321	8289.4	31.281
270.00	58.226	13021.	48.225	80.405	8688.7	32.181
273.15	58.560	13205.	48.342	81.083	8943.1	32.741
275.00	58.747	13313.	48.411	81.478	9093.5	33.067
280.00	59.082	13608.	48.599	82.540	9503.5	33.941
285.00	59.529	13904.	48.787	83.590	9918.8	34.803
290.00	59.984	14203.	48.976	84.629	10339.	35.653
295.00	60.444	14504.	49.166	85.658	10765.	36.492
298.15	60.735	14695.	49.287	86.302	11036.	37.015
300.00	60.905	14807.	49.358	86.678	11196.	37.320

 $S_S^0 = 0$  AT ABSOLUTE ZERO

THE SUBSCRIPT S REFERS TO THE STATE IN EQUILIBRIUM WITH SATURATED VAPOR











TABLE 127

## MOLAL THERMODYNAMIC FUNCTIONS FOR TETRADECANE

NORMAL-C<sub>14</sub>H<sub>30</sub>

SOLID AND LIQUID PHASES

T DEG K=273.15+T DEG C

1 CAL=4.1840 JOULES

GRAM MOLECULAR WT.= 198.39520 GRAMS

T DEG K	C <sub>S</sub> CAL DEG MOL	(H <sub>S</sub> -E <sub>0</sub> <sup>C</sup> ) CAL MOL	(H <sub>S</sub> -E <sub>0</sub> <sup>C</sup> )/T CAL DEG MOL	S <sub>S</sub> <sup>0</sup> CAL MOL	-(G <sub>S</sub> -E <sub>0</sub> <sup>C</sup> ) CAL MOL	-(G <sub>S</sub> -E <sub>0</sub> <sup>C</sup> )/T CAL DEG MOL
SOLID TRICLINIC						
0.00	0.000	0.000	0.000	0.000	0.000	0.000
0.00	0.000	0.000	0.000	0.000	0.000	0.000
5.00	0.073	0.091	0.018	0.024	0.030	0.006
10.00	0.583	1.462	0.146	0.195	0.488	0.049
15.00	1.848	7.206	0.480	0.644	2.448	0.163
20.00	3.785	21.067	1.053	1.428	7.488	0.374
25.00	6.130	45.736	1.829	2.519	17.238	0.690
30.00	8.694	82.720	2.757	3.860	33.094	1.103
35.00	11.357	132.86	3.796	5.401	56.175	1.605
40.00	13.988	196.24	4.906	7.090	87.350	2.184
45.00	16.567	272.65	6.059	8.887	127.25	2.828
50.00	19.078	361.80	7.236	10.763	176.35	3.527
55.00	21.480	463.25	8.423	12.695	234.98	4.272
60.00	23.756	576.39	9.607	14.663	303.36	5.056
65.00	25.885	700.56	10.778	16.649	381.63	5.871
70.00	27.881	835.02	11.929	18.641	469.86	6.712
75.00	29.782	979.21	13.056	20.630	568.04	7.574
80.00	31.595	1132.7	14.159	22.610	676.14	8.452
85.00	33.294	1295.0	15.235	24.578	794.12	9.343
90.00	34.866	1465.4	16.282	26.526	921.89	10.243
95.00	36.331	1643.5	17.299	28.450	1059.3	11.151
100.00	37.722	1828.6	18.286	30.350	1206.3	12.063
105.00	39.062	2020.6	19.244	32.223	1362.8	12.979
110.00	40.357	2219.2	20.174	34.070	1528.5	13.896
115.00	41.608	2424.1	21.079	35.892	1703.4	14.813
120.00	42.815	2635.2	21.960	37.688	1887.4	15.728
125.00	43.984	2852.2	22.817	39.460	2080.3	16.642
130.00	45.125	3075.0	23.653	41.207	2282.0	17.554
135.00	46.242	3303.4	24.469	42.931	2492.3	18.462
140.00	47.340	3537.3	25.267	44.633	2711.2	19.366
145.00	48.424	3776.8	26.047	46.313	2938.6	20.266
150.00	49.495	4021.6	26.810	47.973	3174.3	21.162
155.00	50.556	4271.7	27.559	49.613	3418.3	22.054
160.00	51.612	4527.1	28.294	51.235	3670.4	22.940
165.00	52.666	4787.8	29.017	52.839	3930.6	23.822
170.00	53.722	5053.8	29.728	54.427	4198.8	24.699
175.00	54.783	5325.0	30.429	55.999	4474.9	25.571
180.00	55.852	5601.6	31.120	57.558	4758.8	26.438
185.00	56.934	5883.6	31.803	59.103	5050.4	27.300
190.00	58.031	6171.0	32.479	60.635	5349.8	28.157
195.00	59.147	6463.9	33.148	62.157	5656.7	29.009
200.00	60.286	6762.5	33.812	63.669	5971.3	29.857
205.00	61.451	7066.8	34.472	65.172	6293.4	30.700
210.00	62.649	7377.0	35.129	66.667	6623.0	31.538
215.00	63.884	7693.4	35.783	68.156	6960.1	32.372
220.00	65.164	8016.0	36.436	69.639	7304.6	33.203
225.00	66.495	8345.1	37.089	71.118	7656.5	34.029
230.00	67.884	8681.0	37.744	72.595	8015.7	34.851
235.00	69.338	9024.0	38.400	74.070	8382.4	35.670
240.00	70.863	9374.5	39.060	75.546	8756.4	36.485
245.00	72.465	9732.8	39.726	77.023	9137.9	37.297
250.00	74.148	10099.4	40.397	78.504	9526.7	38.107
255.00	75.917	10474.6	41.076	79.990	9922.9	38.913
260.00	77.774	10859.0	41.764	81.482	10327.0	39.718
265.00	79.721	11252.0	42.462	82.981	10738.0	40.520
270.00	81.758	11656.0	43.170	84.490	11156.0	41.320
273.15	83.089	11916.0	43.623	85.446	11424.0	41.823
275.00	83.887	12070.0	43.891	86.010	11583.0	42.119
279.03	85.668	12412.0	44.481	87.243	11932.0	42.762
LIQUID PHASE						
279.03	102.76	23184.0	83.086	125.85	11932.0	42.762
280.00	102.86	23283.0	83.155	126.20	12054.0	43.050
285.00	103.40	23799.0	83.505	128.03	12690.0	44.525
290.00	103.93	24317.0	83.853	129.83	13334.0	45.980
295.00	104.47	24838.0	84.198	131.61	13988.0	47.417
298.15	104.81	25168.0	84.414	132.73	14404.0	48.312
300.00	105.00	25362.0	84.540	133.37	14650.0	48.835

 $S_S^0 = 0$  AT ABSOLUTE ZERO

THE SUBSCRIPT S REFERS TO THE STATE IN EQUILIBRIUM WITH SATURATED VAPOR





TABLE 130

## MOLAL THERMODYNAMIC FUNCTIONS FOR TETRAPHOSPHORUS DECASULFIDE

 $P_{4S_{10}}$   
 SOLID PHASE

T DEG K=273.15+T DEG C

1 CAL=4.1840 JOULES

GRAM MOLECULAR WT.= 444.5352 GRAMS

T DEG K	$C_p^0$ CAL DEG MOL	$(H_T^0 - H_0^C)$ CAL	$(H_T^0 - H_0^C) / T$ CAL DEG MOL	$S_T^0$ CAL DEG MOL	$-(G_T^0 - H_0^C)$ CAL	$-(G_T^0 - H_0^C) / T$ CAL DEG MOL
0.00	0.000	0.000	0.000	0.000	0.000	0.000
5.00	0.283	0.363	0.073	0.097	0.123	0.025
10.00	1.635	4.750	0.475	0.652	1.769	0.177
15.00	3.589	17.675	1.178	1.673	7.425	0.495
20.00	5.677	40.865	2.043	2.993	18.999	0.950
25.00	7.694	74.298	2.972	4.477	37.625	1.505
30.00	9.744	117.86	3.929	6.060	63.931	2.131
35.00	11.874	171.89	4.911	7.721	98.353	2.810
40.00	14.083	236.76	5.919	9.450	141.26	3.531
45.00	16.307	312.74	6.950	11.238	192.95	4.288
50.00	18.521	399.81	7.996	13.070	253.71	5.074
55.00	20.724	497.93	9.053	14.939	323.72	5.886
60.00	22.879	606.97	10.116	16.835	403.14	6.719
65.00	24.908	726.50	11.177	18.748	492.10	7.571
70.00	26.818	855.85	12.226	20.664	590.62	8.437
75.00	28.706	994.65	13.262	22.578	698.73	9.316
80.00	30.596	1142.9	14.286	24.492	816.41	10.205
85.00	32.415	1300.5	15.300	26.402	943.64	11.102
90.00	34.094	1466.8	16.298	28.303	1080.4	12.005
95.00	35.641	1641.2	17.276	30.188	1226.6	12.912
100.00	37.104	1823.1	18.231	32.054	1382.3	13.823
105.00	38.527	2012.2	19.164	33.808	1547.1	14.735
110.00	39.929	2208.3	20.076	35.723	1721.2	15.647
115.00	41.308	2411.4	20.960	37.528	1904.3	16.559
120.00	42.659	2621.4	21.845	39.315	2096.5	17.470
125.00	43.975	2838.0	22.704	41.083	2297.5	18.380
130.00	45.249	3061.0	23.546	42.833	2507.3	19.287
135.00	46.478	3290.4	24.373	44.564	2725.8	20.191
140.00	47.660	3525.7	25.184	46.276	2952.9	21.092
145.00	48.798	3766.2	25.979	47.968	3188.5	21.990
150.00	49.894	4013.7	26.758	49.641	3432.5	22.883
155.00	50.950	4265.8	27.521	51.294	3684.9	23.773
160.00	51.970	4523.1	28.269	52.928	3945.4	24.659
165.00	52.955	4785.4	29.003	54.543	4214.1	25.540
170.00	53.909	5052.6	29.721	56.138	4490.9	26.417
175.00	54.833	5324.5	30.425	57.714	4775.5	27.288
180.00	55.722	5600.9	31.116	59.271	5067.9	28.155
185.00	56.598	5881.7	31.793	60.810	5368.1	29.017
190.00	57.440	6166.8	32.457	62.331	5576.8	29.874
195.00	58.256	6456.1	33.108	63.833	5991.4	30.725
200.00	59.046	6749.3	33.747	65.318	6314.7	31.571
205.00	59.812	7046.5	34.373	66.786	6644.6	32.413
210.00	60.553	7347.4	34.988	68.236	6982.1	33.248
215.00	61.273	7652.0	35.591	69.669	7326.9	34.079
220.00	61.971	7960.1	36.182	71.086	7678.8	34.904
225.00	62.650	8271.6	36.763	72.486	8037.7	35.723
230.00	63.312	8586.6	37.333	73.870	8403.6	36.537
235.00	63.957	8924.7	37.893	75.239	8776.4	37.346
240.00	64.586	9226.1	38.442	76.592	9156.0	38.150
245.00	65.230	9550.6	38.982	77.930	9542.3	38.948
250.00	65.779	9879.1	39.512	79.253	9935.3	39.741
255.00	66.382	10229.0	40.033	80.562	10335.	40.529
260.00	66.949	10542.	40.546	81.857	10741.	41.311
265.00	67.501	10878.	41.049	83.137	11153.	42.088
270.00	68.036	11217.	41.544	84.404	11572.	42.860
275.00	68.365	11432.	41.851	85.195	11839.	43.344
280.00	68.555	11558.	42.030	85.657	11997.	43.627
285.00	69.544	12249.	42.979	88.124	12866.	45.145
290.00	70.015	12598.	43.441	89.337	13310.	45.896
295.00	70.472	12949.	43.895	90.538	13760.	46.643
298.15	70.752	13171.	44.177	91.288	14046.	47.111
300.00	70.914	13302.	44.342	91.726	14215.	47.384
310.00	71.763	14016.	45.213	94.065	15144.	48.853
320.00	72.568	14738.	46.055	96.356	16096.	50.301
330.00	73.338	15467.	46.870	98.601	17071.	51.731
340.00	74.079	16204.	47.660	100.80	18068.	53.142
350.00	74.794	16949.	48.425	102.96	19087.	54.535

 $H_0^C$  AND  $S_0^C$  APPLY TO THE REFERENCE STATE OF THE SOLID AT ZERO DEG K

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